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Comment on "Collapse of Coherent Quasiparticle States in θ-(BEDT-TTF)$_2$I$_3$ Observed by Optical Spectroscopy"

Recently, Takenaka *et al.*[1] reported that the resistivity $\rho(T)$ of θ-(BEDT-TTF)$_2$I$_3$ (θ-ET) exceeds the Ioffe-Regel resistivity, ρ_{IR}, by a factor of 50 at large temperatures T ("bad metal"). This was ascribed to strong correlation. We argue that the optical conductivity $\sigma(\omega)$ implies that correlation is not very strong, and that correlation gives no general strong suppression of $\sigma(\omega)$. The large $\rho(T)$ is primarily due to a downturn in $\sigma(\omega)$ at small ω, earlier emphasized by Takenaka *et al.* [2] as the explanation for bad metal behavior of high-T_c cuprates. We argue, however, that for cuprates strong correlation is the main effect. The data of Takenaka *et al.*[1] puts θ-ET in a new class of bad metals.

To put θ-ET into context, we discuss a theory of resistivity saturation [3]. We use an f-sum rule, relating $\int \sigma(\omega)d\omega$ to the electron hopping energy, E_K. We assume that T is so large that the Drude peak is smeared out and that $\sigma(\omega)$ varies smoothly over the band width W (shown for Nb$_3$Sb in Fig. 1). We obtain

$$\sigma(0) = \frac{\gamma}{W}\int_0^\infty \sigma(\omega)d\omega \sim \frac{|E_K|}{W}, \qquad (1)$$

where $\gamma \sim 1-2$. Assuming i) noninteracting electrons and ii) $T \ll W$, we estimate E_K. Inserting E_K in Eq. (1) gives $\sigma(0)$ and a quantum-mechanical derivation of the Ioffe-Regel condition, $l \gtrsim d$, where l is the apparent mean free path and d is a typical atomic separation [3].

Assumption i) is invalid for cuprates, and correlation drastically reduces $|E_K|$. Estimating E_K, we obtained the saturation resistivity $\rho_{\rm sat}$ for La$_{2-x}$Sr$_x$CuO$_4$ (LSCO) [3]. Experimental data do not exceed $\rho_{\rm sat}$, and $\rho(T,x)$ curves approaching $\rho_{\rm sat}$ appear to saturate. Fig. 1 shows that strong correlation reduces $\sigma(0)$ of LSCO (x=0.06, T=295 K) by a factor of four relative to $1/\rho_{IR}$, with room for further reduction to $1/\rho_{\rm sat}$ with increasing T.

Assumption ii) is invalid for A$_3$C$_{60}$ (A=K, Rb). This leads to a violation of the Ioffe-Regel condition due to coupling to intramolecular phonons [3].

For the quarter-filled θ-ET, data for $\int \sigma(\omega)d\omega \sim E_K$ for small T suggest that correlation does not strongly reduce $|E_K|$, in strong contrast to cuprates. As a result, $\sigma(\omega)\rho_{IR} \sim 1$, comparable to Nb$_3$Sb, except for very small ω. As in the cuprates, there is a downturn in $\sigma(\omega)$ at small ω ("dynamical localization"). While this is a small effect in cuprates, reducing $\sigma(0)$ by about 10-20 % in Fig. 1 (compared with dashed line), the θ-ET data [1] imply a reduction of $\rho(T$=295) by a factor of 50-100. Thus the absence of such a downturn is a third assumption (iii) for deriving the Ioffe-Regel condition, putting θ-ET in a third class of bad metals. The small energy scale of the downturn, $\sim T$, raises questions why the structure is not thermally smeared out.

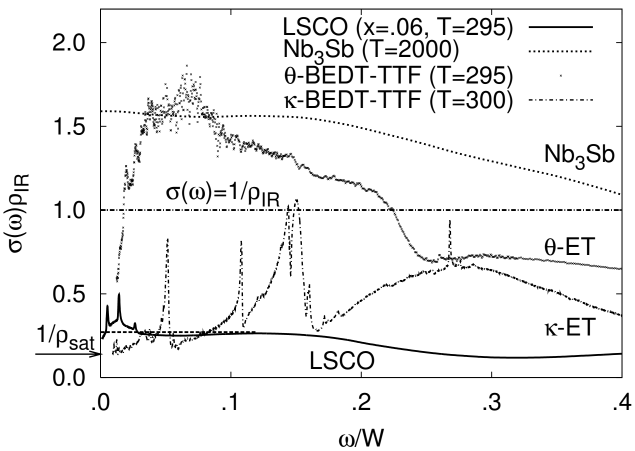

FIG. 1: $\sigma(\omega)\rho_{IR}$ as a function of ω/W for Nb$_3$Sb (theory) [3], LSCO [2], θ-ET [1] and κ-ET [4], where (the noninteracting) W is 8, 3.2, 0.7 and 1.0 (unrealistically large to show all main features) eV, respectively. The interband transitions of LSCO for $\omega/W \gtrsim 0.3$ and sharp phonon structures are not of interest here. The dashed curve indicates a $\sigma(\omega)$ of LSCO without downturn. The Ioffe-Regel condition implies $\sigma(0)\rho_{IR} \gtrsim 1$. All systems are fully in the incoherent limit.

Calculations [3] for A$_3$C$_{60}$, emphasizing coupling to phonons, show that as T is increased $\int_0^{\omega_m}\sigma(\omega)d\omega$ is reduced and reaches its limiting value for larger ω_m. This is similar to θ-ET but very different from cuprates (cf. Fig. 4 in Ref. 1 and inset of Fig. 2 in Ref. 2), suggesting a role for phonons in θ-ET.

Fig. 1 shows that $\sigma(\omega)\rho_{IR}$ is suppressed for the "half-filled" (BEDT-TTF)$_2$Cu[N(CN)$_2$]Br$_{0.85}$Cl$_{0.15}$ (κ-ET) due to correlation reducing $|E_K|$ and expanding the energy scale. There is also a downturn, although less dramatic and on a larger energy scale than for θ-ET . Thus both assumptions i) and iii) are moderately violated.

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